On an inhomogeneous Schrödinger equation and its solutions in scattering theory

van Haeringen, H

Published in:
Journal of Mathematical Physics

DOI:
10.1063/1.524132

On an inhomogeneous Schrödinger equation and its solutions in scattering theory

H. van Haeringen

Natuurkundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands and Institute for Theoretical Physics, P.O. Box 800, University of Groningen, The Netherlands

(Received 19 July 1978)

We prove that $\psi_{s,l}$, the partial-wave projection of the irregular Coulomb wavefunction ψ_s, is a solution of an inhomogeneous Schrödinger equation. New expressions for $\psi_{s,l}$ and ψ_s are obtained in terms of the Coulomb Green functions $G_{C,l}$ and G_C, respectively. We discuss irregular solutions, the analogs of ψ_s, for Coulomb-like and short-range potentials. We find that in general these functions do not approach asymptotically the scattering amplitude times an outgoing spherical wave, in contrast to the pure Coulomb function ψ_s.

1. INTRODUCTION

The physical three-dimensional Coulomb scattering wavefunction $\psi^{(+)}$ is customarily split up into an "incoming part" ψ_i and a "scattered part" ψ_s. Each one of these three functions is a solution of the Schrödinger equation, $\psi^{(+)}$ is regular, ψ_i and ψ_s are irregular. In Ref. 1 we have derived closed expressions for $\psi_l^{(+)}, \psi_{i,l}$, and $\psi_{s,l}$, the partial wave (p.w.) projections of $\psi^{(+)}$, ψ_i, and ψ_s, respectively. We proved that $\psi_{i,l}$ and $\psi_{s,l}$ are *no* solutions of the p.w. projected Schrödinger equation.

The function ψ_s asymptotically approaches the Coulomb scattering amplitude times a Coulomb-modified outgoing spherical wave [cf. Eq. (5.1)]. The question arises whether there also exists for other potentials a function which

(i) is an irregular solution of the three-dimensional Schrödinger equation, and

(ii) asymptotically approaches the scattering amplitude times an outgoing spherical wave (possibly modified).

In this paper we shall discuss a large class of irregular solutions of the three-dimensional Schrödinger equation with a local potential. Their asymptotic behavior is easily obtained when the potential is spherically symmetric. In this case we are able to show that the condition (ii) is not satisfied in general. It seems that the *pure* Coulomb potential is a remarkable exception in this respect.

In Sec. 2 we shall prove that $\psi_{s,l}$ is a solution of an "inhomogeneous Schrödinger equation," see Eq. (2.3). With the help of this result we deduce in Sec. 3 a new expression for $\psi_{s,l}$, in terms of the Coulomb Green function $G_{c,l}$, Eq. (3.1). In the second part of Sec. 3 we investigate the behavior of $\psi_{s,l}(r)$ for $r \to 0$, starting from different equivalent expressions. When $l = 0$ this function diverges like $\ln r$, but for $l > 0$ it has a finite limit for $r \to 0$ [Eq. (3.17)].

Summation of the p.w. series with $\psi_{s,l}$ leads in a natural way to an expression for $\psi_s(\mathbf{k},\mathbf{r})$ in terms of the three-dimensional Coulomb–Green function G_C, Eq. (4.1). We define in Eq. (4.2) a class of irregular solutions $\psi_w(\mathbf{k},\mathbf{r})$ of the three-dimensional Schrödinger equation for a not necessarily spherically symmetric potential in analogy to ψ_s, and study these functions in Sec. 4. We also discuss here the connection with a line charge distribution on the positive z axis.

The most interesting feature of the Coulomb irregular solution ψ_s is, as we said before, that it asymptotically approaches a Coulomb-modified outgoing spherical wave times the Coulomb scattering amplitude. In Sec. 5 we discuss the question whether such an irregular solution with a similar asymptotic behavior can be found for other potentials. We successively consider the Coulomb, Coulomb-like, and short-range potentials, first with the "Coulomb-choice" for w, i.e., $w(r)$ proportional to e^{ikr}, and afterwards for other functions w. We have not been able to find an irregular solution ψ_w with the desired property of giving the scattering amplitude, so it seems to be fortuitous that ψ_s yields asymptotically the scattering amplitude. Therefore, although the regular physical wavefunction $\psi^{(+)}(\mathbf{k},\mathbf{r})$ for any local potential can be expressed as the sum of two irregular solutions, $\psi^{(+)} = \psi_i + \psi_s$, this splitting seems to be useful only in the pure Coulomb case.

We shall work throughout in the coordinate representation and restrict ourselves to local potentials. As usual we take $\hbar = 2m = 1$, $E = (k + i\epsilon)^2$ with $\epsilon \downarrow 0$, and we suppress the energy dependence of G, G_0, and T. We will often use the subscript C to denote Coulomb quantities.

The p.w. "outgoing" physical scattering state is denoted by $|kl+\rangle$, cf. Eq. (11.13) of Taylor.[2] Its connection with Newton's $\psi_l^{(+)}$ and φ_l follows from

$$\langle r|kl+\rangle = (2/\pi)^{1/2}(kr)^{-1} i^l \psi_l^{(+)}(k,r) \tag{1.1}$$

and [Eq. (12.145) of Ref. 3]

$$\psi_l^{(+)}(k,r) = k^{l+1}\varphi_l(k,r) f_l^{-1}(k)/(2l+1)!!, \tag{1.2}$$

where $f_l(k)$ is the Jost function. Furthermore we will use the symbols $|kl\uparrow\rangle$ and $|kl\downarrow\rangle$ to denote the Jost solutions of the p.w. Schrödinger equation, see Ref. 1. We have

$$\langle r|kl\uparrow\rangle = (2/\pi)^{1/2}(kr)^{-1} f_l(k,r), \tag{1.3}$$

$$2i|kl+\rangle = e^{2i\delta_l}|kl\uparrow\rangle - |kl\downarrow\rangle, \tag{1.4}$$

and

$$\langle r|kl+\rangle = (-)^l \langle r|kl-\rangle^* = (-)^l \langle kl-|r\rangle. \tag{1.5}$$

The Coulomb Jost solution is denoted by $\langle r|kl\uparrow\rangle_C$, and for

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$V \equiv 0$ we have[1]

$$\langle r|kl\uparrow\rangle_0 = (2/\pi)^{1/2} i^l h_l^{(+)}(kr). \quad (1.6)$$

We shall suppress l when $l=0$. In particular,

$$\langle r|k\,0\uparrow\rangle_0 = \langle r|k\uparrow\rangle_0 = (2/\pi)^{1/2} e^{ikr}/(kr).$$

The subscript 0 to a bra or ket signifies $V=0$, whereas for a function, e.g., in $f^*_{C,0}$, it means $l=0$. The behavior of $\langle r|kl+\rangle$ and $\langle r|kl\uparrow\rangle$ at $r=0$ follows from

$$\lim_{r\to 0}(\pi/2)^{1/2}(2ikr)^{-l}\langle r|kl+\rangle(2l+1)!!/l!$$
$$= f_l^{-1}(k) \quad (1.7)$$

and

$$\lim_{r\to 0}(\pi/2)^{1/2}(-2ikr)^l kr\langle r|kl\uparrow\rangle l!/(2l)!$$
$$= f_l(k), \quad (1.8)$$

respectively. These equations are valid for Coulomb-like as well as for (nonsingular) short-range potentials.

For a local central potential $V_l(r)$ is independent of l. Therefore, we shall occasionally suppress the subscript l here.

2. COULOMB FUNCTIONS SATISFYING AN INHOMOGENEOUS SCHRÖDINGER EQUATION

In this section we shall prove that χ_l (see Ref. 1) is a solution of the following inhomogeneous differential equation of the Schrödinger type,

$$(k^2 - H_{C,l})\chi_l(kr) = -\langle r|V_C|k\uparrow\rangle_0 f^*_{C,0}, \quad (2.1a)$$

that is, written in a more explicit form,

$$\left(k^2 + \frac{1}{r}\frac{d^2}{dr^2}r - \frac{l(l+1)}{r^2} - \frac{2k\gamma}{r}\right)\chi_l(kr)$$
$$= -\frac{2k\gamma}{r}\left(\frac{2}{\pi}\right)^{1/2}\frac{e^{ikr}}{kr}\frac{e^{\pi\gamma/2}}{\Gamma(1-i\gamma)}. \quad (2.1b)$$

Here V_C is the Coulomb potential and $f^*_{C,0}$ is the complex conjugate of the Coulomb Jost function for $l=0$ (e.g., Ref. 3),

$$f_{C,l} = f_{C,l}(k) = e^{\pi\gamma/2}\Gamma(l+1)/\Gamma(l+1+i\gamma).$$

The function χ_l has been defined in Ref. 1 by

$$\chi_l(kr) = e^{2i\sigma_l}\langle r|kl\uparrow\rangle_C - 2i\psi_{s,l}(r), \quad (2.2)$$

where $\langle r|kl\uparrow\rangle_C$ is the Jost solution for the p.w. Schrödinger equation with the Coulomb potential. It follows that if Eq. (2.1) is valid, we also have

$$(k^2 - H_{C,l})\psi_{s,l}(r) = \langle r|V_C|k\uparrow\rangle_0 f^*_{C,0}/(2i). \quad (2.3)$$

As we said in the Introduction, $\psi_{s,l}$ is the p.w. projection of ψ_s [see Eq. (4) of Ref. 1],

$$\psi_s(\mathbf{k},\mathbf{r}) = -(2\pi)^{-(3/2)}e^{\pi\gamma/2}(\Gamma(1+i\gamma)/\Gamma(-i\gamma))$$
$$\times e^{ikr}U(1+i\gamma,1,i\mathbf{k}\cdot\mathbf{r} - ikr). \quad (2.4)$$

In order to prove Eq. (2.1), we substitute the following closed expression for χ_l [see Eq. (A.17) of Ref. 1],

$$\chi_l(kr) = (2/\pi)^{1/2}\frac{\exp(\pi\gamma/2)}{\Gamma(1-i\gamma)}\frac{\exp(ikr)}{kr}$$
$$\times {}_2F_1\left(-l, l+1, 1; 1-i\gamma; \frac{1}{2ikr}\right), \quad (2.5)$$

and introduce the new variables $z = (2ikr)^{-1}$ and $\mu = -i\gamma$. After some manipulations the equation to be proved reduces to

$$-z^3F''(z) + z(1-2z)F'(z) + [\mu + l(l+1)z]F(z) = \mu. \quad (2.6)$$

Here

$$F(z) \equiv {}_2F_1(-l, l+1, 1; \mu+1; z)$$
$$= \sum_{n=0}^{l} z^n(-l)_n(l+1)_n/(\mu+1)_n$$

is a polynomial, so the proof of Eq. (2.6) is obtained in a straightforward way.

3. A NEW EXPRESSION FOR $\psi_{s,l}$

In this section we shall prove the equation

$$G_{C,l}V_{C,l}|k\uparrow\rangle_0 f^*_{C,0} = 2i\psi_{s,l}, \quad (3.1)$$

where

$$2i\psi_{s,l} = e^{2i\sigma_l}|kl\uparrow\rangle_C - \chi_l. \quad (3.2)$$

The left-hand side of (3.1) gives a new expression for $\psi_{s,l}$. Further we shall investigate the behavior of $\psi_{s,l}(k,r)$ for $r\to 0$, see Eq. (3.17).

Note, however, that

$$G_{C,l}V_{C,l}|k\downarrow\rangle_0$$

is even not defined. This can be easily deduced from our discussion below [the integral $\int_r^\infty$ in Eq. (3.8) would be divergent in this case], but it also follows from the equality $G_{C,l}V_{C,l} = G_{0,l}T_{C,l}$ and the well-known fact that the half-shell Coulomb T matrix, that is $T_{C,l}|kl\rangle$, is not defined.

For the proof of Eq. (3.1) we use

$$\langle r|G_{C,l}|r'\rangle = (-)^{l+1}\tfrac{1}{2}\pi k\langle r_<|kl+\rangle\langle r_>|kl\uparrow\rangle, \quad (3.3)$$

where $r_<$ is the smaller one and $r_>$ the larger one of the pair r,r'. Such a representation of the Green function holds for any local central potential, as is well known.

A natural and direct way to prove Eq. (3.1) would consist of inserting (3.3) and using the known explicit expressions for the regular and irregular Coulomb wavefunctions, i.e.,

$$\langle r|kl+\rangle_C = (2/\pi)^{1/2}e^{-\pi\gamma/2}[\Gamma(l+1+i\gamma)/\Gamma(2l+2)]$$
$$\times(2ikr)^l e^{-ikr}\,{}_1F_1(l+1-i\gamma; 2l+2; 2ikr),$$
$$(3.4a)$$

and

$$\langle r|kl\uparrow\rangle_C=(2/\pi)^{1/2}e^{\pi\gamma/2+ikr}(kr)^{-1}(-2ikr)^{l+1}$$

$$\times U(l+1+i\gamma,2l+2,-2ikr). \qquad (3.4b)$$

However, it turns out that this approach is somewhat complicated. We have been able to prove Eq. (3.1) in this way only for $l=0$ and for $l=1$. In order to show the complications arising here, we now briefly discuss the $l=0$ case. By using

$$\frac{d}{dz}\,{}_1F_1(-i\gamma;1;z)=-i\gamma\ {}_1F_1(1-i\gamma;2;z),$$

$$\frac{d}{dz}e^{-z}U(1+i\gamma,1,z)=-e^{-z}U(1+i\gamma,2,z),$$

and

$${}_1F_1(-i\gamma;1;z)$$
$$=-i\gamma\ {}_1F_1(1-i\gamma;2;z)+(1+i\gamma)\ {}_1F_1(-i\gamma;2;z),$$
$$U(1+i\gamma,1,z)$$
$$=U(1+i\gamma,2,z)-(1+i\gamma)U(2+i\gamma,2,z),$$

we obtain

$$\langle r|G_CV_C|k\uparrow\rangle_0$$
$$=e^{\pi\gamma/2}\Gamma(1+i\gamma)\langle r|k\uparrow\rangle_C+(2/\pi)^{1/2}2ie^{ikr}\Gamma(1+i\gamma)$$
$$\times[{}_1F_1(-i\gamma;1;2ikr)U(1+i\gamma,2,-2ikr)$$
$$+i\gamma\ {}_1F_1(1-i\gamma;2;2ikr)U(1+i\gamma,1,-2ikr)]. \qquad (3.5)$$

The expression between the square brackets can be reduced by noting that the Wronskian W for the functions

$$f(z)\equiv{}_1F_1(-i\gamma;1;z)$$

and

$$g(z)\equiv e^zU(1+i\gamma,1,-z)$$

is equal to

$$W(f,g)\equiv fg'-f'g=z^{-1}\exp[z+i\pi\,\mathrm{sgn}(\mathrm{Im}z)]/\Gamma(1+i\gamma).$$

In this way we get from Eq. (3.5),

$$\langle r|G_CV_C|k\uparrow\rangle_0f^*_{C,0}=e^{2i\sigma_0}\langle r|k\uparrow\rangle_C$$
$$-(2/\pi)^{1/2}e^{\pi\gamma/2}(kr)^{-1}e^{ikr}/\Gamma(1-i\gamma),$$

which is just Eq. (3.1) for $l=0$.

For $l>1$ the above procedure is rather complicated. Therefore, we resort to a different approach.

In the preceding section we have proved

$$(k^2-H_{C,l})(2i\psi_{s,l})=V_C|k\uparrow\rangle_0f^*_{C,0}. \qquad (3.6)$$

This equation follows from Eq. (3.1), but not vice versa. We shall nevertheless prove Eq. (3.1) with the help of Eq. (3.6). To this end we first observe that the quantity $G_{C,l}V_C|k\uparrow\rangle_0f^*_{C,0}$ is a solution of the same inhomogeneous differential equation,

$$(k^2-H_{C,l})G_{C,l}V_C|k\uparrow\rangle_0f^*_{C,0}=V_C|k\uparrow\rangle_0f^*_{C,0}.$$

Therefore, this quantity equals the sum of a particular solution of this equation and some solution of the corresponding homogeneous differential equation. According to Eq. (2.1), $-\chi_l$ is a particular solution. Further, we know that any solution of the homogeneous differential equation is a linear combination of $|kl\uparrow\rangle_C$ and $|kl\downarrow\rangle_C$. Therefore,

$$G_{C,l}V_C|k\uparrow\rangle_0f^*_{C,0}=-\chi_l+C_1|kl\uparrow\rangle_C+C_2|kl\downarrow\rangle_C. \qquad (3.7)$$

We shall prove that $C_2=0$ and $C_1=e^{2i\sigma_l}$ by establishing the behavior of the left-hand side for $r\to\infty$ and for $r\to0$, respectively.

Substitution of (3.3) in the left-hand side of Eq. (3.7) yields

$$\langle r|G_{C,l}V_C|k\uparrow\rangle_0f^*_{C,0}$$
$$=(-)^{l+1}\tfrac{1}{2}\pi kf^*_{C,0}\Big[\langle r|kl\uparrow\rangle_C\int_0^r\langle r'|kl+\rangle_C\ V_C(r')$$
$$\times\langle r'|k\uparrow\rangle_0r'^2dr'+\langle r|kl+\rangle_C\int_r^\infty\langle r'|kl\uparrow\rangle_C$$
$$\times V_C(r')\langle r'|k\uparrow\rangle_0r'^2dr'\Big]. \qquad (3.8)$$

We further use Eq. (1.4) for the Coulomb case,

$$2i|kl+\rangle_C=e^{2i\sigma_l}|kl\uparrow\rangle_C-|kl\downarrow\rangle_C$$

and

$$\langle r|kl\uparrow\rangle_C\sim(2/\pi)^{1/2}(kr)^{-1}\exp[ikr-i\gamma\ln(2kr)],\quad r\to\infty. \qquad (3.9)$$

It follows that for $r\to\infty$ the second term on the right-hand side of Eq. (3.8) is negligible. For the first term we find, for $r\to\infty$,

$$-(2/\pi)^{1/2}f^*_{C,0}(kr)^{-1}e^{ikr}+\text{const }r^{-1-i\gamma}e^{ikr}.$$

Clearly this implies that we have $C_2=0$ in Eq. (3.7).

In order to prove $C_1=e^{2i\sigma_l}$, we consider the expressions in Eq. (3.8) for $r\to0$. With the help of Eqs. (1.7) and (1.8) one easily verifies that

$$\langle r|G_{C,l}V_C|k\uparrow\rangle_0=O(\ln r),\qquad r\to0,\text{when}\ l=0,$$
$$=O(1),\quad r\to0,\text{when}\ l=1,2,3,\cdots. \qquad (3.10)$$

Finally we use Eq. (3.4b), where (Ref. 4, p. 288, corrected)

$$U(a,c,z)=z^{1-c}\Gamma(c-1)/\Gamma(a)+O(|z|^{2-\mathrm{Re}c}),$$
$$z\to0,\ \mathrm{Re}c\geqslant2,\ c\neq2, \qquad (3.11)$$

and deduce from Eq. (26) of Ref. 1 that

$$\chi_l(kr)\simeq(2/\pi)^{1/2}e^{\pi\gamma/2}(kr)^{-1}$$
$$\times(-2ikr)^{-l}\Gamma(2l+1)/\Gamma(l+1-i\gamma),\quad r\to0. \qquad (3.12)$$

With the help of these expressions we obtain $C_1=e^{2i\sigma_l}$. This completes the proof of Eq. (3.1).

The behavior of $\langle r|G_{C,l}V_C|k\uparrow\rangle_0$ at $r\to0$, as given by Eq. (3.10) is somewhat peculiar. The function $\psi_{s,l}$ has the same behavior, according to Eq. (3.1), that has just been proved. It may be interesting to deduce this behavior of $\psi_{s,l}$ at $r=0$ in an independent manner. We shall do this in two ways: (i) by starting from $\psi_s(\mathbf{k},\mathbf{r})$, and (ii) by using an integral representation for $\psi_{s,l}$ which we have obtained previously.[1] These considerations give at the same time a more precise expression for $\psi_{s,l}$ at $r=0$.

First we note that Eqs. (3.2) and (3.4b) may be used for our purpose, but this approach is not simple for $l>0$. So let us start with $\psi_s(\mathbf{k},\mathbf{r})$, a closed form for which has already been given in Eq. (2.4). By using

$$U(1+i\gamma,1,z)\simeq -(2C+\psi(1+i\gamma)+\ln z)/\Gamma(1+i\gamma),\quad z\to 0, \tag{3.13}$$

where C is Euler's constant and ψ the digamma function, we get

$$\psi_s(\mathbf{k},\mathbf{r})\simeq(2\pi)^{-(3/2)}\exp(ikr+\pi\gamma/2)\times\ln(kr-\mathbf{k}\cdot\mathbf{r})/\Gamma(-i\gamma),\quad kr-\mathbf{k}\cdot\mathbf{r}\to 0. \tag{3.14}$$

The p.w. projection of ψ_s is given by

$$\psi_{s,l}(r)\equiv 2\pi\int_{-1}^{1}P_l(x)\psi_s(\mathbf{k},\mathbf{r})dx,$$

with $x=\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}$. We now use the equalities

$$\begin{aligned}\int_{-1}^{1}P_l(x)\ln(1-x)dx &= 2\ln 2-2,\quad l=0\\ &= -2/[l(l+1)],\quad l=1,2,3,\cdots,\end{aligned} \tag{3.15}$$

that follow easily with the help of (e.g., Ref. 4, p. 239)

$$\sum_{n=1}^{\infty}(n^{-1}+(n+1)^{-1}P_n(x) = -1+\ln 2-\ln(1-x),\quad -1\leqslant x<1. \tag{3.16}$$

In this way we obtain, for $r\to 0$,

$$\begin{aligned}(\pi/2)^{1/2}e^{-\pi\gamma/2}\Gamma(-i\gamma)\psi_{s,l}(r)&\simeq\ln r,\quad l=0\\ &\simeq -1/[l(l+1)],\\ l=1,2,3\cdots.\end{aligned} \tag{3.17}$$

This expression not only agrees with Eq. (3.10) but also gives more information.

Finally we will deduce the expression (3.17) from the following integral representation for $\psi_{s,l}$ [Eq. (18) of Ref. 1],

$$\psi_{s,l}(r)=-(2/\pi)^{1/2}i^{-l}e^{\pi\gamma/2}[\Gamma(-i\gamma)]^{-1}\times\int_0^\infty j_l(krt)e^{ikr(1+t)}t^{i\gamma}(1+t)^{-1-i\gamma}dt. \tag{3.18}$$

We use the new variable $z=krt$ and see that we have to investigate the following integral for small r,

$$I_l(r)\equiv\int_0^\infty j_l(z)e^{iz}(z+kr)^{-1}(1+kr/z)^{-i\gamma}dz. \tag{3.19}$$

When $l>0$ we may put $r=0$ in the integrand because of $j_l(z)=O(z^l)$, $z\to 0$. In this case we obtain

$$\lim_{r\to 0}I_l(r)=\int_0^\infty j_l(z)e^{iz}z^{-1}dz=i^l/[l(l+1)],\quad l=1,2,3,\cdots, \tag{3.20}$$

which follows by using formula 6.621.1 of Ref. 5. For $l=0$ we have

$$\begin{aligned}I_0(r)+\ln kr &= \int_0^\infty \sin z e^{iz}z^{-1}(z+kr)^{-1}(1+kr/z)^{-i\gamma}dz\\ &\quad-\int_0^{1-kr}(z+kr)^{-1}dz,\end{aligned}$$

which clearly has a finite limit for $r\to 0$, so

$$I_0(r)=-\ln kr+O(1),\quad r\to 0. \tag{3.21}$$

By substituting the above results in Eq. (3.18) we obtain the second proof of Eq. (3.17).

4. IRREGULAR SOLUTIONS IN THE GENERAL CASE

In the preceding section we have expressed $\psi_{s,l}$ in terms of the Coulomb Green function $G_{C,l}$, see Eq. (3.1). By summing the p.w. series for both sides of this equation we obtain

$$\psi_s(\mathbf{k},\mathbf{r})=\int_0^\infty\langle\mathbf{r}|G_C|\hat{\mathbf{k}}r'\rangle V_C(r')\langle r'|k\uparrow\rangle_0 r'^2dr'f^*_{C,0}/(2i). \tag{4.1}$$

In this section we shall discuss irregular solutions ψ_w for a general potential V, not necessarily spherically symmetric. To this end we define, in close analogy to Eq. (4.1),

$$\psi_w(\mathbf{k},\mathbf{r})\equiv\int_0^\infty\langle\mathbf{r}|G|\hat{\mathbf{k}}r'\rangle w(r')dr', \tag{4.2}$$

where $G=(k^2+\Delta-V)^{-1}$ and the function w is arbitrary to the extent that the above integral is well defined. For convenience we assume w to be continuously differentiable. By a formal application of G^{-1} it is easily seen that ψ_w satisfies

$$(k^2+\Delta-V)\psi_w(\mathbf{k},\mathbf{r})=r^{-2}w(r)\delta(\hat{\mathbf{r}},\hat{\mathbf{k}}). \tag{4.3}$$

The Dirac delta function is defined by

$$\int f(\hat{\mathbf{r}})\delta(\hat{\mathbf{r}},\hat{\mathbf{k}})d\hat{\mathbf{r}}=f(\hat{\mathbf{k}}),$$

where the domain of integration is the surface of the unit sphere.

We will show that ψ_w in general has a logarithmic singularity in the forward direction ($\hat{\mathbf{k}}=\hat{\mathbf{r}}$). By inserting $G=G_0+G_0VG$ in (4.2) one can show that this singularity in general comes from G_0. So we replace G by G_0 in Eq. (4.2) and use

$$\langle\mathbf{r}|G_0|\mathbf{r}'\rangle=-(4\pi)^{-1}|\mathbf{r}-\mathbf{r}'|^{-1}\exp(ik|\mathbf{r}-\mathbf{r}'|).$$

It follows that the singular part of ψ_w is given by

$$\psi_w=-(4\pi)^{-1}\int_0^\infty w(r')\exp(iky)/ydr'+O(1),\quad x\to 1,$$

with $y=(r^2+r'^2-2rr'x)^{1/2}$ and $x=\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}$ as before. The singularity comes from the integrand at the point $r'=r$. In order to investigate its behavior in this region we introduce the new variable $z = r'/r$. Then one can show that for any positive a,

$$\int_a^1 (1 - 2xz + z^2)^{-1/2} f(z)dz = \mp \tfrac{1}{2} f(1)\ln(1-x) + O(1), \quad x\uparrow 1, \quad a \lessgtr 1, \tag{4.4}$$

for a continuously differentiable function $f(z)$. With the help of Eq. (4.4) we obtain

$$\psi_w = (4\pi)^{-1} w(r)\ln(1-x) + O(1), \quad x\uparrow 1. \tag{4.5}$$

This expression gives the logarithmic singularity of the irregular solution ψ_w for a general local potential V.

Now we will briefly discuss the singular behavior of ψ_w at $r = 0$. In this case we assume $x \neq 1$. Since $(z^2 - 2xz + 1)^{1/2} \sim z$ for $z \to \infty$ we have

$$\psi_w = -(4\pi)^{-1} \int_1^\infty e^{ikrz} w(rz)\frac{dz}{z} + O(1), \quad r \to 0. \tag{4.6}$$

When w is constant we use

$$\Gamma(0, -ikr) = \int_1^\infty e^{ikrz}\frac{dz}{z} = -\ln kr + O(1), \quad r \to 0,$$

where Γ is the incomplete gamma function, and obtain from Eq. (4.6),

$$\psi_w = (4\pi)^{-1} w(0)\ln kr + O(1), \quad r \to 0. \tag{4.7}$$

When w is proportional to e^{ikr} [cf. Eq. (4.13)] we get exactly the same expression, (4.7).

We note that Eqs. (4.5) and (4.7) can be combined,

$$\psi_w(\mathbf{k},\mathbf{r}) = (4\pi)^{-1} w(r)\ln(kr - \mathbf{k}\cdot\mathbf{r}) + O(1), \tag{4.8}$$

for $\hat{\mathbf{k}}\cdot\hat{\mathbf{r}} \to 1$ as well as for $r \to 0$. This expression may be compared with Eq. (3.14).

If we now restrict ourselves to spherically symmetric potentials, $\psi_w(\mathbf{k},\mathbf{r})$ is a function of k, r and $\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}$ only. In this case it is possible to consider the p.w. projection of (4.2),

$$\psi_{w,l}(k,r) = \int_0^\infty \langle r|G_l|r'\rangle w(r')dr'. \tag{4.9}$$

In order to deduce the behavior of $\psi_{w,l}$ at $r = 0$, we use Eq. (3.3) which is valid for any local central potential. Then Eq. (4.9) may be rewritten as

$$\psi_{w,l}(k,r) = (-)^{l+1}\tfrac{1}{2}\pi k \left[\langle r|kl\uparrow\rangle \int_0^r \langle r'|kl+\rangle w(r')dr' + \langle r|kl+\rangle \int_r^\infty \langle r'|kl\uparrow\rangle w(r')dr'\right]. \tag{4.10}$$

By using Eqs. (1.7) and (1.8) we obtain

$$\psi_{w,l}(k,r) \simeq -(2l+1)^{-1} w(0)\left[r^{-l-1}\int_0^r r'^l dr' + r^l \int_r^{r_0} r'^{-l-1}dr'\right], \quad r \to 0, \tag{4.11}$$

where r_0 is an unimportant constant. Therefore,

$$\psi_{w,l}(k,r) = w(0)\ln r + O(1), \quad r\to 0, \quad l = 0,$$
$$= -w(0)/[l(l+1)] + o(1), \quad r \to 0, \quad l = 1,2,3,\cdots. \tag{4.12}$$

One easily verifies that the p.w. projection of both sides of Eq. (4.8) yields expressions for $\psi_{w,l}$ that are in agreement with Eq. (4.12).

We note that for the Coulomb case, $G = G_C$, ψ_w is just equal to the irregular Coulomb wave ψ_s given by Eq. (2.4) if we choose the function w as

$$w(r) = -i\gamma(2/\pi)^{1/2} f^*_{C,0} e^{ikr}. \tag{4.13}$$

We conclude this section with a remark on the logarithmic singularity of ψ_w, given by Eq. (4.8). We see from Eq. (4.3) that the delta function singularity must be generated by the Laplace operator acting on $\ln(kr - \mathbf{k}\cdot\mathbf{r})$, so

$$\Delta \ln(kr - \mathbf{k}\cdot\mathbf{r}) \simeq 4\pi r^{-2}\delta(\hat{\mathbf{r}},\hat{\mathbf{k}}). \tag{4.14}$$

It is interesting to note that one can verify that Eq. (4.14) holds with an equality sign.

In order to show this, let us take $\hat{\mathbf{k}}$ along the positive z-axis as before. Then the right-hand side of (4.14) describes a uniform line charge density along the positive z-axis. In view of the symmetry in the problem it is natural to use cylindrical coordinates R, z, φ, where $R^2 = r^2 - z^2$. Then we have

$$2\pi r^{-2}\delta(\hat{\mathbf{r}},\hat{\mathbf{z}}) = r^{-2}\delta(1-\cos\zeta) = R^{-1}\delta(R)\theta(z),$$

where θ is the unit step function. Further,

$$kr - \mathbf{k}\cdot\mathbf{r} = k(r-z) = k((R^2+z^2)^{1/2} - z).$$

The electrostatic potential for a uniform charge distribution on the positive z axis is just proportional to the logarithmic term discussed above. Poisson's equation reads in this case

$$\Delta \ln((R^2+z^2)^{1/2} - z) = 2R^{-1}\delta(R)\theta(z). \tag{4.15}$$

This equation shows that (4.14) holds with an equality sign. So we see that the inhomogeneous term in Eq. (4.3) may be compared with a line charge distribution along the positive z axis with density $w(r)$ or $w(z)$.

5. ON THE CONNECTION WITH THE SCATTERING AMPLITUDE

The function $\psi_s(\mathbf{k},\mathbf{r})$ [see Eq. (2.4)] is called the scattered part of the complete physical scattering wavefunction $\psi^{(+)}(\mathbf{k},\mathbf{r})$ for the Coulomb potential because of its asymptotic behavior, which is given by [cf. Eq. (40) of Ref. 1]

$$\psi_s(\mathbf{k},\mathbf{r}) \sim f^C(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})(2\pi)^{-(3/2)} r^{-1}\exp(ikr - i\gamma\ln 2kr), \quad r \to \infty. \tag{5.1}$$

Here f^C is the Coulomb scattering amplitude,

$$f^C(x) = -\frac{\gamma}{2k} e^{2i\sigma_0}(\tfrac{1}{2} - \tfrac{1}{2}x)^{-1-i\gamma}.$$

One may compare (5.1) with the well-known short-range potential formula,

$$\psi^{(+)}(\mathbf{k},\mathbf{r}) \sim (2\pi)^{-3/2}(e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)e^{ikr}/r), \quad r \to \infty.$$

From Eq. (4.1).

$$\psi_s(\mathbf{k},\mathbf{r}) = \int_0^\infty \langle \mathbf{r}|G_C|\hat{\mathbf{k}}r'\rangle V_C(r')\langle r'|k\uparrow\rangle_0 r'^2 dr' f^*_{C,0}/(2i),$$

we see that this "scattered part" equals an integral involving the Green operator G_C.

It is interesting to investigate whether Eq. (4.1) can be generalized to other potentials. The problem is, how to find an irregular solution, such that its asymptotic behavior equals the scattering amplitude times a (possibly modified) outgoing spherical wave, just as in Eq. (5.1).

Let us first consider again the p.w. function $\psi_{s,l}$ for the pure Coulomb potential. Below we shall consider the generalization to Coulomb-like and other potentials. From Eqs. (3.1) and (3.8) we have, for $r\to\infty$,

$$\psi_{s,l}(k,r)\sim\tfrac{1}{4}i\pi k f^*_{C,0}\langle r|kl\uparrow\rangle_C\int_0^r {}_C\langle kl-|r'\rangle \times V_C(r')\langle r'|k\uparrow\rangle_0 r'^2dr'. \tag{5.2}$$

We split the integral in two parts, $\int_0^R+\int_R^r$, where R is so large that the asymptotic behavior of ${}_C\langle kl-|r'\rangle$ can be used. With the help of Eqs. (1.4) and (3.9) we obtain a term with the asymptotic behavior $-(2/\pi)^{1/2}f^*_{C,0}e^{ikr}/(2ikr)$. According to Eq. (3.2),

$$\psi_{s,l}(k,r)=(-\chi_l+e^{2i\sigma_l}\langle r|kl\uparrow\rangle_C)/(2i),$$

this term is $-\chi_l/(2i)$. The rest of $\psi_{s,l}$ is proportional to $\langle r|kl\uparrow\rangle_C$. By using Eq. (3.1) we deduce

$$e^{2i\sigma_l}=f^*_{C,0}\lim_{R\to\infty}\left[(2kR)^{i\gamma}-\tfrac{1}{2}\pi k\int_0^R {}_C\langle kl-|r\rangle V_C(r)\times\langle r|k\uparrow\rangle_0 r^2dr\right]. \tag{5.3}$$

It is interesting to replace $\langle r|k\uparrow\rangle_0$ by $\langle r|q\uparrow\rangle_0$ here, where as before

$$\langle r|q\uparrow\rangle_0=(2/\pi)^{1/2}e^{iqr}/(qr),$$

with $\operatorname{Im}q>0$ and consider the limit for $q\to k$. When $q\neq k$ the integral $\int_0^R\cdots$ is convergent for $R\to\infty$ and may be denoted in this case by ${}_C\langle kl-|V_{C,l}|q\uparrow\rangle_0$. We have been able to obtain the following closed expressions,

$$\begin{aligned}{}_C\langle kl-|V_{C,l}|q\uparrow\rangle_0 &=\frac{4i\gamma}{\pi q}e^{\pi\gamma/2}\left(\frac{q+k}{q-k}\right)^{i\gamma/2}Q_l^{i\gamma}(q/k)\\ &=-\frac{2}{\pi q}e^{-\pi\gamma/2}\frac{\Gamma(1+i\gamma)\Gamma(1-i\gamma)\Gamma(l+1)}{\Gamma(l+1-i\gamma)}\\ &\quad\times\left[P_l^{(i\gamma,-i\gamma)}(q/k)-\left(\frac{q+k}{q-k}\right)^{i\gamma}P_l^{(-i\gamma,i\gamma)}(q/k)\right].\end{aligned} \tag{5.4}$$

Here $Q_l^{i\gamma}$ is Legendre's function of the second kind, and $P_l^{(\cdot,\cdot)}$ is Jacobi's polynomial. In the particular case $l=0$ this expression agrees with Eq. (7) of Ref. 6 that we used for the derivation of the Coulomb off-shell Jost function in closed form.

When $q\sim k$, Eq. (5.4) can be simplified. By inserting

$$P_l^{(i\gamma,-i\gamma)}(1)=\Gamma(l+1+i\gamma)/[\Gamma(1+i\gamma)\Gamma(l+1)], \tag{5.5}$$

we obtain

$${}_C\langle kl-|V_{C,l}|q\uparrow\rangle_0\underset{q\to k}{\sim}-\frac{2}{\pi k}e^{-\pi\gamma/2}\left[e^{2i\sigma_l}\Gamma(1-i\gamma)-\Gamma(1+i\gamma)\left(\frac{q+k}{q-k}\right)^{i\gamma}\right]. \tag{5.6}$$

The second term on the right-hand side contains the factor $(q-k)^{-i\gamma}$ and is therefore singular for $q\to k$. It may be compared with the "correction factor" ω of Ref. 6, Eq. (2). Note also the similarity with the so-called Coulombian asymptotic state of Ref. 7, Eq. (16), where the typical factor $f^*_{C,0}(p+k)^{i\gamma}(p-k)^{-i\gamma}$ occurs.

This singular term corresponds to that part of the integral on the right-hand side of Eq. (5.3) which contains the (for $R\to\infty$) divergent factor $(2kR)^{i\gamma}$. The other term is continuous for $q\to k$ and this one corresponds just to the "convergent part" of the integral in (5.3).

A natural generalization of the expression $\langle r|G_{C,l}V_{C,l}|k\uparrow\rangle_0$ to other central potentials is

$$\psi_l(k,r)\equiv\langle r|G_lV_l|k\uparrow\rangle_0, \tag{5.7}$$

where G_l is the Green function for V_l. So ψ_l corresponds to the Coulomb function $\psi_{s,l}$ of Eq. (3.1) [we have omitted the constant factor $f^*_{C,0}/(2i)$ which is irrelevant here]. We first assume that V_l is a Coulomb plus short-range potential, $V_{C,l}+V_{s,l}$. In order to investigate the asymptotic behavior of ψ_l, we use the expression [cf. Eq. (3.3)]

$$\langle r|G_l|r'\rangle=-\tfrac{1}{2}\pi k\langle kl-|r_<\rangle\langle r_>|kl\uparrow\rangle.$$

It may be noted that $\langle r|kl\uparrow\rangle$ has exactly the same asymptotic behavior as $\langle r|kl\uparrow\rangle_C$, which is given by Eq. (3.9). Furthermore we have [cf. Eq. (1.4)]

$$2i\langle kl-|=\exp[2i(\sigma_l+\delta_l^C)]\langle kl\downarrow|-\langle kl\uparrow|, \tag{5.8}$$

where δ_l^C is the Coulomb-modified phase shift. We proceed in the same way as in the pure Coulomb case, and find that ψ_l can again be split up in two parts, $\psi_l=\psi_l^{(1)}+\psi_l^{(2)}$, which have different asymptotic behavior. For the first term we get

$$\psi_l^{(1)}(r)\sim-(2/\pi)^{1/2}e^{ikr}/(kr),\quad r\to\infty,\quad l=0,1,2,\ldots. \tag{5.9}$$

Obviously this is the analog of the function χ_l. Since the right-hand side of (5.9) is independent of l, it follows that the sum of the p.w. series,

$$\sum_{l=0}^{\infty}(4\pi)^{-1}(2l+1)P_l(x)\psi_l^{(1)}(r),$$

is proportional to $\delta(1-x)$ for $r\to\infty$.

For the second term we obtain

$$\psi_l^{(2)}(r)\sim\langle r|kl\uparrow\rangle\lim_{R\to\infty}\left[(2kR)^{i\gamma}-\tfrac{1}{2}\pi k\int_0^R\langle kl-|r'\rangle V(r')\langle r'|k\uparrow\rangle_0 r'^2dr'\right],\quad r\to\infty. \tag{5.10}$$

The integral $\int_0^R$ is divergent for $R \rightarrow \infty$. In this limit it has exactly the same singular behavior as for the pure Coulomb case, which can be verified with the help of Eq. (5.8). It is therefore natural to split off the pure Coulomb part. We do this by using the two-potential formalism; in the notation of Ref. 8 we have

$$V_l|kl+\rangle = V_{C,l}|kl+\rangle_C + (1+T_{C,l}G_{0,l})t_{Cs,l}|kl+\rangle_C, \tag{5.11a}$$

or

$$\langle kl-|V_l = {}_C\langle kl-|V_{C,l} + {}_C\langle kl-|t_{Cs,l}(1+G_{0,l}T_{C,l}). \tag{5.11b}$$

Here $t_{Cs,l}$ satisfies the equation

$$t_{Cs,l} = V_{s,l} + V_{s,l}G_{C,l}t_{Cs,l},$$

so it is a "short-range operator." Substitution of (5.11) in (5.10) yields

$$\psi_l^{(2)}(r) \sim \langle r|kl\uparrow\rangle[f_{C,0}^{*\,-1}e^{2i\sigma_l} - \tfrac{1}{2}\pi k_C\langle kl-| \times t_{Cs,l}(1+G_{0,l}T_{C,l})|k\uparrow\rangle_0], \tag{5.12}$$

where we have used Eq. (5.3). The phase shift for $V_{C,l}+V_{s,l}$ is related to $t_{Cs,l}$ in the following well-known way,

$${}_C\langle kl-|t_{Cs,l}|kl+\rangle_C = i(\pi k)^{-1}e^{2i\sigma_l}[\exp(2i\delta_l^C)-1]. \tag{5.13}$$

Comparison with Eq. (5.12) shows that the p.w. series $\Sigma_l(4\pi)^{-1}(2l+1)P_l(x)\psi_l^{(2)}(r)$ is not proportional to the scattering amplitude in general. Therefore, also

$$\psi(\mathbf{k},\mathbf{r}) = \sum_{l=0}^{\infty}(4\pi)^{-1}(2l+1)P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})\psi_l(r)$$

does not in general have the desired asymptotic behavior [recall that the p.w. series with $\psi_l^{(1)}$ is proportional to $\delta(1-x) = \delta(1-\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})$, for $r\rightarrow\infty$].

For a short-range potential we obtain for $r\rightarrow\infty$, following the same procedure,

$$\psi_l(r) \sim -\tfrac{1}{2}\pi k\langle r|kl\uparrow\rangle\langle kl-|V_l|k\uparrow\rangle_0 = -\tfrac{1}{2}\pi k\langle r|kl\uparrow\rangle\langle kl|T_l|k\uparrow\rangle_0. \tag{5.14}$$

In this case the phase shift δ_l is given by

$$\langle kl|T_l|kl\rangle = i(\pi k)^{-1}(e^{2i\delta_l}-1).$$

Apparently the p.w. series with the ψ_l of (5.14) will in general not be proportional to the scattering amplitude, for $r\rightarrow\infty$.

The procedure described above can be repeated for the function $\psi_{w,l}$ of Sec. 4. That is, we replace $\langle r|k\uparrow\rangle_0$ by a rather arbitrary function $w(r)$ and consider the asymptotic behavior of $\psi_{w,l}(r)$, see Eq. (4.9). Again we are not able to find a function w for any potential (except for V_C), such that $\psi_w(\mathbf{k},\mathbf{r})$ for $r\rightarrow\infty$ approaches the scattering amplitude times an outgoing spherical wave.

So it seems that the pure Coulomb function ψ_s in unique in having the property (5.1). This would mean that the useful property (5.1) of the irregular solution ψ_s is merely a coincidence. Therefore, although the regular physical wavefuntion $\psi^{(+)}(\mathbf{k},\mathbf{r})$ for any potential can be expressed as the sum of two irregular solutions $\psi^{(+)} = \psi_i + \psi_s$, this splitting seems to be useful only in the pure Coulomb case.

ACKNOWLEDGMENT

This investigation forms a part of the research program of the Foundation for Fundamental Research of Matter (FOM), which is financially supported by the Netherlands Organization for Pure Scientific Research (ZWO).

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